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5-(3,4-Dimethoxyphenyl)-1-(4-methylphenyl)pyrazolidin-3-one

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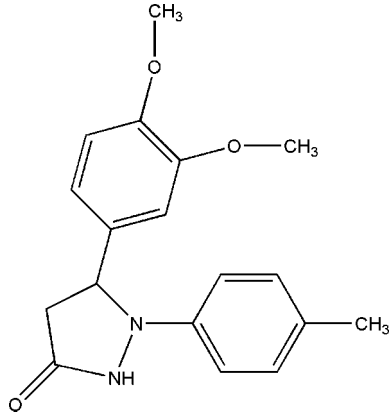
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.076; wR factor = 0.187; data-to-parameter ratio = 16.2.

In the molecule of the title compound, $C_{18}H_{20}N_2O_3$, the five-membered ring adopts an envelope conformation. Intramolecular C—H···N hydrogen bonds cause the formation of two further five-membered planar rings. In the crystal structure, intermolecular C—H···O and N—H···O hydrogen bonds link the molecules to form a three-dimensional network.

Related literature

For general background, see: Menozzi *et al.* (1990); Brooks *et al.* (1990); Greenwood *et al.* (1995). For related literatue, see: Zhu *et al.* (2004). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{18}H_{20}N_2O_3$
M_r = 312.36
Triclinic, $P\overline{1}$
a = 9.4290 (19) Å
b = 10.107 (2) Å
c = 10.848 (2) Å
α = 96.50 (3)°
β = 111.60 (3)°
γ = 114.43 (3)°
V = 831.0 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 298 (2) K
0.40 × 0.30 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.965, T_{max} = 0.982
3477 measured reflections
3266 independent reflections
2256 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
3 standard reflections
frequency: 120 min
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.076
$wR(F^2)$ = 0.187
S = 1.05
3266 reflections
202 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.54 e Å^{-3}
$\Delta\rho_{min}$ = −0.75 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O3^{i}	0.86	2.00	2.836 (5)	163
C1—H1A···O3^{ii}	0.96	2.57	3.472 (6)	156
C13—H13A···O2^{iii}	0.93	2.52	3.452 (5)	176
C5—H5A···N1	0.93	2.49	2.846 (5)	103
C17—H17A···N2	0.93	2.43	2.755 (5)	101

Symmetry codes: (i) $-x+1, -y, -z+2$; (ii) $x+1, y+1, z+1$; (iii) $-x+1, -y+1, -z+3$.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1985); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2301).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Brooks, D. W., Basha, A., Gunn, B. P. & Bhatia, P. A. (1990). US Patent No. 4 970 210.
Bruker (2000). *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Enraf–Nonius (1985). *CAD-4 Software*. Version 5.0. Enraf–Nonius, Delft, The Netherlands.
Greenwood, B., Helton, D. R. & Howbert, J. J. (1995). US Patent No. 5 399 565.
Harms, K. & Wocadlo, S. (1995). *XCAD4*. University of Marburg, Germany.
Menozzi, G., Mosti, L. & Schenone, P. (1990). *Il Farmaco*, **45**, 167–186.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Zhu, H.-J., Ma, J., Wei, C.-M. & Wang, J.-T. (2004). *Acta Cryst.* E**60**, o411–o413.

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supplementary materials

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5-(3,4-Dimethoxyphenyl)-1-(4-methylphenyl)pyrazolidin-3-one

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Comment

Pyrazolidin-3-one derivatives are of great interest because of their biological properties, such as antipyretic activity (Menozzi *et al.*, 1990), liphoxygenase enzyme inhibition (Brooks *et al.*, 1990) and cholecystokinin (CCK) receptor antagonist activity (Greenwood *et al.*, 1995). In the process of synthesis, we obtained the title compound, (I), and we herein report its crystal structure.

In the molecule of the title compound, (I), (Fig. 1) the bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The intramolecular C—H···N hydrogen bonds (Table 1) cause to the formation of two five-membered planar rings A (N1/C9/C6/C5/H5A) and B (N2/N1/C12/C17/H17A). The five-membered ring C (N1/N2/C9—C11) is not planar and has an envelope conformation with atom C9 is displaced by −0.470 (3) Å from the plane of the other ring atoms. D (C3—C8) and E (C12—C17) rings are, of course, planar and the dihedral angles between the planar rings are A/B = 83.84 (2)°, A/D = 1.65 (3) and B/E = 2.22 (3)°.

In the crystal structure, intermolecular C—H···O and N—H···O hydrogen bonds (Table 1) link the molecules to form a three-dimensional network (Fig. 2). The intra- and intermolecular hydrogen bonds seem to be effective in the stabilization of the crystal structure.

Experimental

To a solution of sodium (40 mmol) in anhydrous methanol (9 ml) was added ethanolamine (4 ml) and n-butanol (20 ml). The methanol was removed by distillation and ethyl 3-(3,4-dimethoxyphenyl)acrylate (9.4 g) was added. The resulting mixture was refluxed for 1 h at 373 K, then 4-methylphenylhydrazine (4.9 g) was added. The reaction mixture was refluxed for a further 6 h, left to cool to room temperature, acidified with acetic acid (36%), allowed to stand, filtered, and the filter cake was crystallized from ethanol to give the title compound (m.p. 412 K). Crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an ethanol solution (Zhu *et al.*, 2004).

Refinement

H atoms were positioned geometrically with N—H = 0.86 Å (for NH), C—H = 0.93, 0.98, 0.97 and 0.96 Å for aromatic, methine, methylene and methyl H atoms, respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = xU_{eq}(C,*N*), where x = 1.5 for methyl H, and x = 1.2 for all other H atoms.

Figures

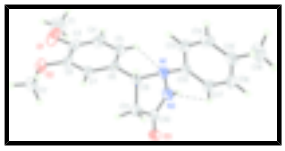

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 40% probability level. Hydrogen bonds are shown as dashed lines.

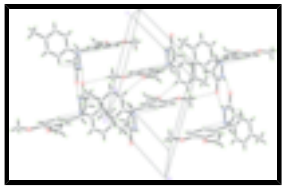

Fig. 2. A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

5-(3,4-Dimethoxyphenyl)-1-(4-methylphenyl)pyrazolidin-3-one

Crystal data

$C_{18}H_{20}N_2O_3$	$Z = 2$
$M_r = 312.36$	$F_{000} = 332$
Triclinic, $P\overline{1}$	$D_x = 1.248$ Mg m^{-3}
Hall symbol: -P 1	Melting point: 412 K
$a = 9.4290$ (19) Å	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$b = 10.107$ (2) Å	Cell parameters from 25 reflections
$c = 10.848$ (2) Å	$\theta = 10$–13°
$\alpha = 96.50$ (3)°	$\mu = 0.09$ mm^{-1}
$\beta = 111.60$ (3)°	$T = 298$ (2) K
$\gamma = 114.43$ (3)°	Block, colorless
$V = 831.0$ (5) Å^3	0.40 × 0.30 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer	$R_{int} = 0.033$
Radiation source: fine-focus sealed tube	$\theta_{max} = 26.0^\circ$
Monochromator: graphite	$\theta_{min} = 2.1^\circ$
$T = 298$(2) K	$h = -11 \rightarrow 10$
$\omega/2\theta$ scans	$k = -12 \rightarrow 12$
Absorption correction: ψ scan (North *et al.*, 1968)	$l = 0 \rightarrow 13$
$T_{min} = 0.965$, $T_{max} = 0.982$	3 standard reflections
3477 measured reflections	every 120 min
3266 independent reflections	intensity decay: none
2256 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.076$

$wR(F^2) = 0.187$

$S = 1.05$

3266 reflections

202 parameters

Primary atom site location: structure-invariant direct methods

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.05P)^2 + 1.3P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.54$ e Å^{-3}

$\Delta\rho_{min} = -0.75$ e Å^{-3}

Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2$sigma(F^2) is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.9140 (3)	0.7698 (3)	1.6030 (3)	0.0823 (10)
O2	0.6384 (4)	0.7591 (3)	1.4264 (3)	0.0622 (7)
O3	0.4293 (3)	0.1296 (3)	0.9351 (2)	0.0507 (6)
N1	0.3685 (3)	0.0623 (3)	1.2249 (3)	0.0408 (6)
N2	0.4294 (4)	0.0539 (3)	1.1247 (3)	0.0443 (6)
H2A	0.4875	0.0072	1.1242	0.053*
C1	1.0718 (7)	0.7904 (6)	1.6861 (6)	0.102
H1A	1.1489	0.8963	1.7407	0.152*
H1B	1.1188	0.7605	1.6301	0.152*
H1C	1.0613	0.7290	1.7470	0.152*
C2	0.4899 (6)	0.7622 (4)	1.3261 (4)	0.0689 (11)
H2B	0.5106	0.8654	1.3433	0.103*
H2C	0.3871	0.6989	1.3344	0.103*
H2D	0.4729	0.7245	1.2337	0.103*
C3	0.7828 (5)	0.6260 (4)	1.5139 (4)	0.0520 (9)
C4	0.7907 (5)	0.4925 (4)	1.5148 (4)	0.0577 (9)
H4A	0.8916	0.4962	1.5785	0.069*
C5	0.6475 (4)	0.3518 (4)	1.4203 (3)	0.0471 (8)
H5A	0.6528	0.2622	1.4227	0.057*
C6	0.4998 (4)	0.3456 (3)	1.3244 (3)	0.0375 (7)
C7	0.4940 (4)	0.4819 (3)	1.3249 (3)	0.0411 (7)
H7A	0.3935	0.4783	1.2605	0.049*

C8	0.6322 (4)	0.6205 (3)	1.4175 (3)	0.0431 (7)
C9	0.3381 (4)	0.1974 (3)	1.2193 (3)	0.0397 (7)
H9A	0.2375	0.1803	1.2359	0.048*
C10	0.3897 (4)	0.1241 (3)	1.0309 (3)	0.0397 (7)
C11	0.2950 (4)	0.1966 (3)	1.0682 (3)	0.0427 (7)
H11A	0.1697	0.1369	1.0074	0.051*
H11B	0.3374	0.2998	1.0623	0.051*
C12	0.2129 (4)	−0.0769 (3)	1.1967 (3)	0.0391 (7)
C13	0.1462 (5)	−0.0834 (4)	1.2907 (4)	0.0539 (9)
H13A	0.1990	0.0017	1.3679	0.065*
C14	0.0013 (5)	−0.2156 (4)	1.2711 (4)	0.0594 (10)
H14A	−0.0435	−0.2175	1.3347	0.071*
C15	−0.0788 (4)	−0.3457 (4)	1.1586 (4)	0.0502 (8)
C16	−0.0111 (5)	−0.3373 (4)	1.0668 (4)	0.0502 (8)
H16A	−0.0639	−0.4225	0.9897	0.060*
C17	0.1349 (4)	−0.2051 (4)	1.0845 (3)	0.0441 (8)
H17A	0.1794	−0.2035	1.0208	0.053*
C18	−0.2397 (5)	−0.4880 (4)	1.1361 (5)	0.0746 (12)
H18A	−0.2765	−0.5661	1.0541	0.112*
H18B	−0.3322	−0.4651	1.1242	0.112*
H18C	−0.2130	−0.5235	1.2157	0.112*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0469 (15)	0.0648 (18)	0.084 (2)	0.0143 (13)	0.0090 (15)	−0.0226 (15)
O2	0.0804 (18)	0.0322 (12)	0.0575 (15)	0.0212 (12)	0.0256 (14)	0.0059 (11)
O3	0.0699 (16)	0.0443 (13)	0.0469 (13)	0.0281 (12)	0.0347 (12)	0.0180 (11)
N1	0.0494 (15)	0.0334 (13)	0.0480 (15)	0.0201 (12)	0.0298 (13)	0.0165 (12)
N2	0.0559 (16)	0.0431 (15)	0.0554 (17)	0.0305 (13)	0.0366 (14)	0.0250 (13)
C1	0.102	0.102	0.102	0.050	0.047	0.032
C2	0.100 (3)	0.051 (2)	0.055 (2)	0.041 (2)	0.030 (2)	0.0209 (18)
C3	0.048 (2)	0.0449 (19)	0.0448 (19)	0.0137 (16)	0.0198 (16)	−0.0044 (15)
C4	0.046 (2)	0.063 (2)	0.049 (2)	0.0275 (18)	0.0114 (17)	0.0023 (17)
C5	0.0481 (19)	0.0451 (18)	0.0462 (19)	0.0231 (16)	0.0207 (16)	0.0104 (15)
C6	0.0419 (17)	0.0340 (15)	0.0346 (15)	0.0146 (13)	0.0209 (14)	0.0088 (12)
C7	0.0492 (18)	0.0366 (16)	0.0369 (16)	0.0190 (14)	0.0218 (14)	0.0110 (13)
C8	0.0530 (19)	0.0341 (16)	0.0409 (17)	0.0168 (14)	0.0267 (16)	0.0080 (13)
C9	0.0411 (17)	0.0307 (15)	0.0463 (18)	0.0153 (13)	0.0219 (14)	0.0120 (13)
C10	0.0419 (17)	0.0282 (15)	0.0408 (17)	0.0128 (13)	0.0168 (14)	0.0086 (13)
C11	0.0457 (18)	0.0343 (16)	0.0412 (17)	0.0197 (14)	0.0143 (14)	0.0078 (13)
C12	0.0431 (17)	0.0319 (15)	0.0402 (16)	0.0164 (13)	0.0185 (14)	0.0145 (13)
C13	0.065 (2)	0.0410 (18)	0.0421 (18)	0.0117 (17)	0.0296 (17)	0.0066 (15)
C14	0.071 (2)	0.052 (2)	0.053 (2)	0.0188 (19)	0.038 (2)	0.0196 (17)
C15	0.0482 (19)	0.0357 (17)	0.055 (2)	0.0140 (15)	0.0187 (17)	0.0193 (15)
C16	0.054 (2)	0.0315 (16)	0.053 (2)	0.0182 (15)	0.0186 (17)	0.0072 (14)
C17	0.0531 (19)	0.0394 (17)	0.0467 (18)	0.0250 (15)	0.0279 (16)	0.0104 (14)
C18	0.062 (3)	0.049 (2)	0.088 (3)	0.0066 (19)	0.033 (2)	0.026 (2)

Geometric parameters (Å, °)

O1—C1	1.336 (6)	C6—C9	1.521 (4)
O1—C3	1.376 (4)	C7—C8	1.370 (4)
O2—C8	1.369 (4)	C7—H7A	0.9300
O2—C2	1.438 (5)	C9—C11	1.535 (4)
O3—C10	1.226 (4)	C9—H9A	0.9800
N1—N2	1.412 (3)	C10—C11	1.496 (4)
N1—C12	1.446 (4)	C11—H11A	0.9700
N1—C9	1.511 (4)	C11—H11B	0.9700
N2—C10	1.335 (4)	C12—C13	1.376 (4)
N2—H2A	0.8600	C12—C17	1.377 (4)
C1—H1A	0.9600	C13—C14	1.382 (5)
C1—H1B	0.9600	C13—H13A	0.9300
C1—H1C	0.9600	C14—C15	1.387 (5)
C2—H2B	0.9600	C14—H14A	0.9300
C2—H2C	0.9600	C15—C16	1.360 (5)
C2—H2D	0.9600	C15—C18	1.508 (5)
C3—C4	1.383 (5)	C16—C17	1.394 (5)
C3—C8	1.393 (5)	C16—H16A	0.9300
C4—C5	1.399 (5)	C17—H17A	0.9300
C4—H4A	0.9300	C18—H18A	0.9600
C5—C6	1.369 (4)	C18—H18B	0.9600
C5—H5A	0.9300	C18—H18C	0.9600
C6—C7	1.401 (4)		
C1—O1—C3	119.4 (4)	N1—C9—C11	102.6 (2)
C8—O2—C2	117.6 (3)	C6—C9—C11	112.0 (2)
N2—N1—C12	113.3 (2)	N1—C9—H9A	110.2
N2—N1—C9	103.1 (2)	C6—C9—H9A	110.2
C12—N1—C9	112.8 (2)	C11—C9—H9A	110.2
C10—N2—N1	114.9 (2)	O3—C10—N2	125.2 (3)
C10—N2—H2A	122.6	O3—C10—C11	127.6 (3)
N1—N2—H2A	122.6	N2—C10—C11	107.2 (3)
O1—C1—H1A	109.5	C10—C11—C9	103.3 (3)
O1—C1—H1B	109.5	C10—C11—H11A	111.1
H1A—C1—H1B	109.5	C9—C11—H11A	111.1
O1—C1—H1C	109.5	C10—C11—H11B	111.1
H1A—C1—H1C	109.5	C9—C11—H11B	111.1
H1B—C1—H1C	109.5	H11A—C11—H11B	109.1
O2—C2—H2B	109.5	C13—C12—C17	118.9 (3)
O2—C2—H2C	109.5	C13—C12—N1	118.1 (3)
H2B—C2—H2C	109.5	C17—C12—N1	122.9 (3)
O2—C2—H2D	109.5	C12—C13—C14	120.4 (3)
H2B—C2—H2D	109.5	C12—C13—H13A	119.8
H2C—C2—H2D	109.5	C14—C13—H13A	119.8
O1—C3—C4	125.3 (3)	C13—C14—C15	121.4 (3)
O1—C3—C8	114.9 (3)	C13—C14—H14A	119.3
C4—C3—C8	119.8 (3)	C15—C14—H14A	119.3

C3—C4—C5	120.3 (3)	C16—C15—C14	117.4 (3)
C3—C4—H4A	119.8	C16—C15—C18	121.6 (3)
C5—C4—H4A	119.8	C14—C15—C18	121.0 (4)
C6—C5—C4	120.2 (3)	C15—C16—C17	122.1 (3)
C6—C5—H5A	119.9	C15—C16—H16A	118.9
C4—C5—H5A	119.9	C17—C16—H16A	118.9
C5—C6—C7	118.7 (3)	C12—C17—C16	119.8 (3)
C5—C6—C9	123.5 (3)	C12—C17—H17A	120.1
C7—C6—C9	117.8 (3)	C16—C17—H17A	120.1
C8—C7—C6	121.8 (3)	C15—C18—H18A	109.5
C8—C7—H7A	119.1	C15—C18—H18B	109.5
C6—C7—H7A	119.1	H18A—C18—H18B	109.5
O2—C8—C7	126.0 (3)	C15—C18—H18C	109.5
O2—C8—C3	114.9 (3)	H18A—C18—H18C	109.5
C7—C8—C3	119.1 (3)	H18B—C18—H18C	109.5
N1—C9—C6	111.6 (3)		
C12—N1—N2—C10	102.0 (3)	C7—C6—C9—N1	176.2 (2)
C9—N1—N2—C10	−20.3 (3)	C5—C6—C9—C11	−120.1 (3)
C1—O1—C3—C4	9.6 (6)	C7—C6—C9—C11	61.8 (3)
C1—O1—C3—C8	−170.8 (4)	N1—N2—C10—O3	−179.6 (3)
O1—C3—C4—C5	178.9 (3)	N1—N2—C10—C11	2.1 (4)
C8—C3—C4—C5	−0.6 (5)	O3—C10—C11—C9	−161.6 (3)
C3—C4—C5—C6	1.3 (5)	N2—C10—C11—C9	16.7 (3)
C4—C5—C6—C7	−1.2 (5)	N1—C9—C11—C10	−27.6 (3)
C4—C5—C6—C9	−179.3 (3)	C6—C9—C11—C10	92.2 (3)
C5—C6—C7—C8	0.6 (4)	N2—N1—C12—C13	177.5 (3)
C9—C6—C7—C8	178.8 (3)	C9—N1—C12—C13	−65.8 (4)
C2—O2—C8—C7	−2.8 (5)	N2—N1—C12—C17	1.2 (4)
C2—O2—C8—C3	177.5 (3)	C9—N1—C12—C17	117.8 (3)
C6—C7—C8—O2	−179.7 (3)	C17—C12—C13—C14	−1.2 (5)
C6—C7—C8—C3	0.1 (5)	N1—C12—C13—C14	−177.7 (3)
O1—C3—C8—O2	0.1 (4)	C12—C13—C14—C15	1.2 (6)
C4—C3—C8—O2	179.7 (3)	C13—C14—C15—C16	−1.2 (6)
O1—C3—C8—C7	−179.6 (3)	C13—C14—C15—C18	−178.3 (4)
C4—C3—C8—C7	0.0 (5)	C14—C15—C16—C17	1.1 (5)
N2—N1—C9—C6	−91.5 (3)	C18—C15—C16—C17	178.3 (3)
C12—N1—C9—C6	146.0 (2)	C13—C12—C17—C16	1.2 (5)
N2—N1—C9—C11	28.6 (3)	N1—C12—C17—C16	177.5 (3)
C12—N1—C9—C11	−93.9 (3)	C15—C16—C17—C12	−1.2 (5)
C5—C6—C9—N1	−5.8 (4)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2A···O3^{i}	0.86	2.00	2.836 (5)	163
C1—H1A···O3^{ii}	0.96	2.57	3.472 (6)	156
C13—H13A···O2^{iii}	0.93	2.52	3.452 (5)	176
C5—H5A···N1	0.93	2.49	2.846 (5)	103

C17—H17A···N2	0.93	2.43	2.755 (5)	101

Symmetry codes: (i) −*x*+1, −*y*, −*z*+2; (ii) *x*+1, *y*+1, *z*+1; (iii) −*x*+1, −*y*+1, −*z*+3.

Fig. 1

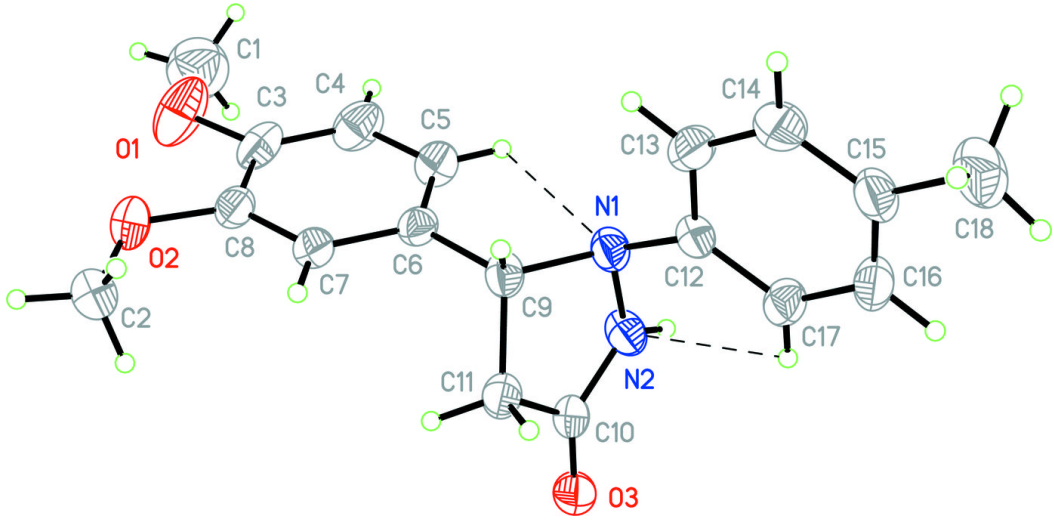

Fig. 2